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Einführung in die Theoretische Festkörperphysik

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Exercise 8

(Due date: 16.12.2019)

Problem 1 (**Tight Binding Model**) (3 points)

Given a single-atom simple cubic crystal with lattice parameter a. In the atomic limit (i.e. considering localized atoms) for each atom n there is only one electronic state $|n\rangle$ with energy E_0. On the other side, in the crystal the orbitals of nearest neighbors overlap (matrix element t).

a) How does the Hamilton operator H of the crystal looks like in the basis $|n\rangle$?
Hint: The complete Hamiltonian is the sum of all atomic Hamiltonians plus the hopping terms.

b) Show that the dispersion relation is given by

$$E(\vec{k}) = E_0 + 2t \sum_{i=1}^{3} \cos(k_i a).$$

Hint: The following representation can be helpful:

$$|\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_n e^{i\vec{k}\vec{R}_n} |n\rangle.$$

c) Consider the case of a 1D chain of atoms with distance a. Calculate and plot the density of states $\mathcal{D}(E)$.

Problem 2 (**Kronig-Penney Model in the Tight Binding Approximation**) (4 points)

We consider a 1D chain of atoms with distance a that generate a potential $V(x) = -g \sum_n \delta(x - na)$.

a) First, solve the atomic problem. Determine the wave function and the corresponding energy dispersion. Plot the wave function for $m = \hbar = g = 1$.

b) Calculate the dispersion relation for the 1D chain in the tight binding approximation considering the atomic wave functions from a).

Problem 3 (**Tight Binding bandstructure**) (3 points)

Determine the energy dispersion $\epsilon(\vec{k})$ of electrons on a 2D triangular lattice considering only nearest neighbor hopping t. Evaluate the density of states $D(E)$ numerically.